Conjugate-Gradient Minimization of the Energy for a 2D Electron under a Magnetic Field

5/29/92

§. Hamiltonian

$$\mathcal{H} = \frac{1}{2m_*}\left(p_x - \frac{m_*\omega_c}{2}y\right)^2 + \frac{1}{2m_*}\left(p_y + \frac{m_*\omega_c}{2}x\right)^2 + v(x,y) \qquad (1)$$

$$= \quad T_x \quad + \quad T_y \quad + \quad V \qquad (2)$$

(Discretization)

$$T_x\psi_{i,j} = \Big(\underbrace{-\frac{\hbar^2}{2m_*\Delta x^2} + \frac{\hbar\omega_c}{4i\Delta x}y_j}_{b_x}\Big)\psi_{i-1,j} + \Big(\underbrace{\frac{\hbar^2}{m_*\Delta x^2} + \frac{m_*\omega_c^2}{8}y_j^2}_{2a_x}\Big)\psi_{i,j}$$
$$+ \Big(\underbrace{-\frac{\hbar^2}{2m_*\Delta x^2} - \frac{\hbar\omega_c}{4i\Delta x}}_{b_x^*}y_j\Big)\psi_{i+1,j} \qquad (3)$$

$$T_y\psi_{i,j} = \Big(\underbrace{-\frac{\hbar^2}{2m_*\Delta y^2} - \frac{\hbar\omega_c}{4i\Delta y}}_{b_y}x_i\Big)\psi_{i,j-1} + \Big(\underbrace{\frac{\hbar^2}{m_*\Delta y^2} + \frac{m_*\omega_c^2}{8}}_{2a_y}x_i^2\Big)\psi_{i,j}$$
$$+ \Big(\underbrace{-\frac{\hbar^2}{2m_*\Delta y^2} + \frac{\hbar\omega_c}{4i\Delta y}}_{b_y^*}x_i\Big)\psi_{i,j+1} \qquad (4)$$

$$V\psi_{ij} = v_{i,j}\,\psi_{i,j} \qquad (5)$$

§. Problem

Minimize an energy functional

$$E[\psi(\mathbf{r})] = \frac{\int d\mathbf{r}\, \psi^*(\mathbf{r})\, h(\mathbf{r})\, \psi(\mathbf{r})}{\int d\mathbf{r}\, |\psi(\mathbf{r})|^2} \tag{6}$$

with a constraint,

$$\int d\mathbf{r}\, |\psi(\mathbf{r})|^2 = 1 \tag{7}$$

§. Gradient (Residual Vector)

$$R(\mathbf{r}) \equiv -\frac{\delta E}{\delta \psi^*(\mathbf{r})}$$

$$= -\frac{h(\mathbf{r})\,\psi(\mathbf{r})}{\langle\psi|\psi\rangle} + \frac{\langle\psi|h|\psi\rangle}{\langle\psi|\psi\rangle^2}\,\psi(\mathbf{r})$$

For a normalized wave function, $\langle\psi|\psi\rangle = 1$,

$$R(\mathbf{r}) = -\frac{\delta E}{\delta \psi^*(\mathbf{r})}$$ → plural float resr & resi

$$= -h(\mathbf{r})\,\psi(\mathbf{r}) + \underbrace{\langle\psi|h|\psi\rangle}_{hpp}\,\psi(\mathbf{r}) \tag{8}$$

§. Conjugate Gradient

[I]

$$Y_n(\mathbf{r}) = \begin{cases} R_0(\mathbf{r}) & (n=0) \\ R_n(\mathbf{r}) + \dfrac{\overbrace{\langle R_n | R_n \rangle}^{\text{gamma1}}}{\underbrace{\langle R_{n-1} | R_{n-1} \rangle}_{\text{gamma0}}} Y_{n-1}(\mathbf{r}) & (n \geq 1) \end{cases} \tag{9}$$

[II]

$$Y_n(\mathbf{r}) = Y_n(\mathbf{r}) - \psi_n(\mathbf{r}) \langle \psi_n | Y_n \rangle \tag{10}$$

[III]

Normalize $\langle Y_n | Y_n \rangle = 1$

§. Line Minimization

Let $\psi(\mathbf{r})$ & $\Upsilon(\mathbf{r})$ be a wave function & a search direction. Suppose $\langle \Upsilon|\psi\rangle = 0$ & $\langle\psi|\psi\rangle = \langle\Upsilon|\Upsilon\rangle = 1$. The following line search conserves the normalization,

$$\psi_\theta(\mathbf{r}) = \cos\theta\,\psi(\mathbf{r}) + \sin\theta\,\Upsilon(\mathbf{r}) \qquad (11)$$

$$E(\theta) = \langle \cos\theta\,\psi + \sin\theta\,\Upsilon | h | \cos\theta\,\psi + \sin\theta\,\Upsilon\rangle$$

$$= \underbrace{\cos^2\theta}_{\frac{1+\cos 2\theta}{2}} \underbrace{\langle\psi|h|\psi\rangle}_{h_{\psi\psi}} + \underbrace{\sin\theta\cos\theta}_{\frac{1}{\cancel{2}}\sin 2\theta} \underbrace{[\langle\psi|h|\Upsilon\rangle + \langle\Upsilon|h|\psi\rangle]}_{2\mathrm{Re}\langle\Upsilon|h|\psi\rangle = \cancel{2}\mathrm{Re}\,h_{\Upsilon\psi}} + \underbrace{\sin^2\theta}_{\frac{1-\cos 2\theta}{2}} \langle\Upsilon|h|\Upsilon\rangle$$

$$E(\theta) = \frac{h_{\psi\psi} + h_{\Upsilon\Upsilon}}{2} + \frac{h_{\psi\psi} - h_{\Upsilon\Upsilon}}{2}\cos 2\theta + \mathrm{Re}\,h_{\Upsilon\psi}\sin 2\theta \qquad (12)$$

$$\frac{\partial E}{\partial\theta} = -(h_{\psi\psi} - h_{\Upsilon\Upsilon})\sin 2\theta + 2\mathrm{Re}\,h_{\Upsilon\psi}\cos 2\theta$$

$$\frac{\partial E}{\partial\theta_{min}} = 0 \quad\rightarrow\quad \theta_{min} = \frac{1}{2}\tan^{-1}\left(\frac{\overbrace{2\mathrm{Re}\,h_{\Upsilon\psi}}^{hyp}}{\underbrace{h_{\psi\psi}}_{hpp} - \underbrace{h_{\Upsilon\Upsilon}}_{hyy}}\right) \qquad (13)$$

$$\tan 2\theta_{min} = \frac{hyp \rightsquigarrow 2\langle y|h|\psi\rangle}{\underbrace{hpp}_{\langle\psi|h|\psi\rangle} - \underbrace{hyy}_{\langle y|h|y\rangle}}$$

Equation (13) gives two solutions

$$\cos 2\theta_{min} = \pm \frac{h_{pp} - h_{yy}}{\sqrt{(h_{pp}-h_{yy})^2 + h_{py}^2}} \qquad \sin 2\theta_{min} = \pm \frac{h_{py}}{\sqrt{(h_{pp}-h_{yy})^2 + h_{py}^2}} \tag{A1}$$

Note that

$$\frac{\partial^2 E}{\partial \theta^2} = -2(h_{\psi\psi} - h_{yy}) \cos 2\theta - 4 \operatorname{Re} h_{y\psi} \sin 2\theta \tag{A2}$$

$$\therefore \frac{\partial^2 E}{\partial \theta_{min}^2} = -2 \left[(h_{pp} - h_{yy}) \cos 2\theta_{min} + 2 h_{py} \sin 2\theta_{min} \right]$$

$$= \mp \frac{2}{\sqrt{(h_{pp}-h_{yy})^2 + h_{py}^2}} \left[(h_{pp}-h_{yy})^2 + 2 h_{py}^2 \right] \tag{A3}$$

We should choose the minus-sign solution in Eq. (A1).

$$\cos 2\theta_{min} = -\frac{h_{pp} - h_{yy}}{\sqrt{(h_{pp}-h_{yy})^2 + h_{yp}^2}} \quad , \quad \sin 2\theta_{min} = \frac{-h_{yp}}{\sqrt{(h_{pp}-h_{yy})^2 + h_{yp}^2}} \tag{14}$$

so that

$$E_{min} = \frac{h_{pp} + h_{yy}}{2} + \frac{-(h_{pp} - h_{yy})^2}{2\sqrt{(h_{pp}-h_{yy})^2 + h_{yp}^2}} + \frac{-h_{yp}^2}{2\sqrt{(h_{pp}-h_{yy})^2 + h_{yp}^2}} \tag{15}$$

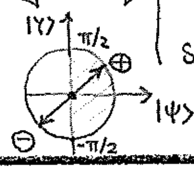
$\oplus$

$$\left\{ \begin{array}{ll} \cos\theta_{min} = \sqrt{\dfrac{1+\cos 2\theta_{min}}{2}} & (16) \\ \sin\theta_{min} = \dfrac{\sin 2\theta_{min}}{2\cos\theta_{min}} & (17) \end{array} \right.$$

equivalent $\longleftrightarrow$

$\ominus$

$$\left\{ \begin{array}{l} \cos\theta_{min} = -\sqrt{\dfrac{1+\cos 2\theta_{min}}{2}} \\ \sin\theta_{min} = \dfrac{\sin 2\theta_{min}}{2\cos\theta_{min}} \end{array} \right.$$



$$E_{min} = \frac{h_{pp} + h_{yy} - \sqrt{(h_{pp}-h_{yy})^2 + h_{yp}^2}}{2}$$

$$\Delta E \equiv E_{min} - h_{pp}$$

$$= \frac{-(h_{pp} - h_{yy}) - \sqrt{(h_{pp}-h_{yy})^2 + h_{yp}^2}}{2} \leq 0 \quad (0 \text{ if } h_{pp} < h_{yy} \ \& \ h_{yp} = 0)$$

§. Algorithm

Initialize $\psi_0(\mathbf{r}) \longrightarrow$ psir & psii

$$\underbrace{R_0(\mathbf{r})}_{\text{resr \& resi}} = -h(\mathbf{r})\psi_0(\mathbf{r}) + \underbrace{h_{\psi_0\psi_0}}_{\text{hpp}}\psi_0(\mathbf{r})$$

$$\gamma_0 = \langle R_0 | R_0 \rangle$$

$$Y_0(\mathbf{r}) = R_0(\mathbf{r}) - \psi_0(\mathbf{r})\langle \psi_0 | R_0 \rangle$$

Normalize $\langle Y_0 | Y_0 \rangle = 1$

do $n = 0$, Ncgmax

calculate $\underbrace{2\mathrm{Re}\,h_{Y_n\psi_n}}_{h_{yp}}$, $\underbrace{h_{Y_nY_n}}_{h_{yy}}$

$$\cos 2\theta_{min} = \frac{h_{pp} - h_{yy}}{\sqrt{(h_{pp}-h_{yy})^2 + h_{yp}^2}} ; \quad \sin 2\theta_{min} = \frac{-h_{yp}}{\sqrt{(h_{pp}-h_{yp})^2 + h_{yp}^2}}$$

$$\cos\theta_{min} = \sqrt{\frac{1+\cos 2\theta_{min}}{2}} ; \quad \sin\theta_{min} = \frac{\sin 2\theta_{min}}{2\cos\theta_{min}}$$

$$\psi_{n+1}(\mathbf{r}) \leftarrow \cos\theta_{min}\,\psi_n(\mathbf{r}) + \sin\theta_{min}\,Y_n(\mathbf{r})$$

$$E_{min} = \frac{h_{pp} + h_{yy}}{2} - \frac{\sqrt{(h_{pp}-h_{yy})^2 + h_{yp}^2}}{2}$$

if ($|E_{min} - h_{pp}| < \epsilon$) exit

$h_{pp} \leftarrow E_{min}$

$\cancel{\gamma_n = \langle R_n | R_n \rangle}$

$$R_{n+1}(\mathbf{r}) = -h(\mathbf{r})\psi_{n+1}(\mathbf{r}) + h_{pp}\psi_{n+1}(\mathbf{r})$$

$$Y_{n+1}(\mathbf{r}) = R_{n+1}(\mathbf{r}) + \frac{\overbrace{\langle R_{n+1} | R_{n+1} \rangle}^{\gamma_{n+1}}}{\gamma_n} Y_n(\mathbf{r})$$

$\underset{\text{gamma0}}{\gamma_n} \leftarrow \underset{\text{gamma1}}{\gamma_{n+1}}$

$$Y_{n+1}(\mathbf{r}) = Y_{n+1}(\mathbf{r}) - \psi_{n+1}(\mathbf{r})\langle \psi_{n+1} | Y_{n+1} \rangle$$

Normalize $\langle Y_{n+1} | Y_{n+1} \rangle = 1$

enddo